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14. ABSTRACT
In this project we focused on the development of theoretical techniques (primarily numerical) that could be used to study correlated topological phases where density functional theory (DFT) could not. The main tool we sought to develop is dynamical mean field theory (DMFT). In DMFT, the main object is the single-particle Green's function. Theoretical work independent of this project established formulas that express the topological properties in terms of the single-particle Greens functions. Thus, there is a direction connection between the quantities that DMFT can compute, and the topological properties of a material. The major technical challenge in DMFT is the so-called

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Report Title

Final Report

ABSTRACT

In this project we focused on the development of theoretical techniques (primarily numerical) that could be used to study correlated topological phases where density functional theory (DFT) could not. The main tool we sought to develop is dynamical mean field theory (DMFT). In DMFT, the main object is the single-particle Green's function. Theoretical work independent of this project established formulas that express the topological properties in terms of the single-particle Greens functions. Thus, there is a direction connection between the quantities that DMFT can compute, and the topological properties of a material. The major technical challenge in DMFT is the so-called "impurity solver". Our main result in this roughly 12-month project was to benchmark various methods of solving the DMFT problem: NCA, OCA, CT-QMC, and IPT. Certain methods are computationally cheaper, but less accurate. We identified some of the tradeoffs in the choices and brought the PI's group capability to the point where it can be applied to the study of strongly interacting topological phases.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
02/27/2013	2.00	Xiang Hu, Andreas Rüegg, Gregory A. Fiete. Topological phases in layered pyrochlore oxide thin films along the [111] direction, Physical Review B, (12 2012): 235141. doi: 10.1103/PhysRevB.86.235141
02/27/2013	3.00	Emanuel Gull, Gregory A. Fiete, Andrew J. Millis, Andreas Rüegg. Sum rule violation in self-consistent hybridization expansions, Physical Review B, (02 2013): 75124. doi: 10.1103/PhysRevB.87.075124
04/22/2013	7.00	Mehdi Kargarian, Gregory A. Fiete. Topological Crystalline Insulators in Transition Metal Oxides, Physical Review Letters, (04 2013): 156403. doi: 10.1103/PhysRevLett.110.156403
04/22/2013	8.00	Hsiang-Hsuan Hung, Lei Wang, Zheng-Cheng Gu, Gregory A. Fiete. Topological phase transition in a generalized Kane-Mele-Hubbard model: A combined quantum Monte Carlo and Green's function study, Physical Review B, (03 2013): 121113. doi: 10.1103/PhysRevB.87.121113
04/23/2014	13.00	Joseph Maciejko, Victor Chua, Gregory Fiete. Topological Order in a Correlated Three-Dimensional Topological Insulator, Physical Review Letters, (01 2014): 16404. doi: 10.1103/PhysRevLett.112.016404
04/23/2014	14.00	Andreas Rüegg, Chandrima Mitra, Alexander A. Demkov, Gregory A. Fiete. Lattice distortion effects on topological phases in (LaNiO_{3})_{2}/(LaAlO_{3})_{N} heterostructures grown along the [111] direction, Physical Review B, (09 2013): 115146. doi: 10.1103/PhysRevB.88.115146
04/23/2014	12.00	Hsiang-Hsuan Hung, Emanuel Gull, Gregory A. Fiete, Andreas Rüegg. Comparative DMFT study of the <math><msub><mi>e</mi><mi>g</mi></msub></math>-orbital Hubbard model in thin films, Physical Review B, (02 2014): 85122. doi: 10.1103/PhysRevB.89.085122
TOTAL:	**7**	

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received		Paper
02/27/2013	4.00	Gregory A. Fiete. Topological insulators: Crystalline protection, Nature Materials, (11 2012): 1003. doi: 10.1038/nmat3473
TOTAL:	**1**	

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper
TOTAL:	

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper
TOTAL:	

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received		Paper
02/27/2013	1.00	Xiang Hu, Andreas Ruegg, Gregory A. Fiete. Topological phases in layered pyrochlore oxide thin films along the [111] direction, arXiv:1211.0562 (11 2012)
02/27/2013	5.00	Mehdi Kargarian, Gregory A. Fiete. Topological Crystalline Insulators in Transition Metal Oxides, arXiv:1212.4162 (12 2012)
02/27/2013	6.00	Hsiang-Hsuan Hung, Lei Wang, Zheng-Cheng Gu, Gregory A. Fiete. Topological phase transition in a generalized Kane-Mele-Hubbard model: A combined Quantum Monte Carlo and Green's function study, Phys Rev Lett (submitted) (02 2013)
08/23/2013	9.00	Joseph Maciejko, Victor Chua, Gregory A. Fiete. Topological order in a correlated three-dimensional topological insulator, ArXiv e-prints (07 2013)
08/23/2013	10.00	Hsiang-Hsuan Hung, Victor Chua, Lei Wang, Gregory A. Fiete. Finite-size and interaction effects on topological phase transitions via numerically exact quantum Monte Carlo calculations, ArXiv e-prints (07 2013)
08/23/2013	11.00	Andreas Ruegg, Chandrima Mitra, Alexandera A. Demkov, Gregory A. Fiete. Strain effects on topological phases in (LaNiO$_3$)$_2$/(LaAlO$_3$)$_N$ heterostructures grown along the [111] direction, ArXiv e-prints (07 2013)
TOTAL:		**6**

Number of Manuscripts:

Books

Received		Paper
TOTAL:		

Patents Submitted

Patents Awarded

Awards

DARPA Young Faculty Award
Tenure!

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Qi Chen	0.60	
FTE Equivalent:	**0.60**	
Total Number:	**1**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Hsiang-Hsuan	1.00
FTE Equivalent:	**1.00**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Greg Fiete	0.05	
FTE Equivalent:	**0.05**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

The goal of this project was to study interacting systems with topological properties using techniques beyond density functional theory, which is only appropriate for weakly interacting electrons. The project was expected to last 2 years (DARPA was providing the money), but the sequester reduced the length to only 1 year. In the period the grant was active, the PI made good progress towards to the overall goals. Most importantly, this project allowed the PI to establish the necessary techniques in his group--namely dynamical mean field theory (DMFT). Dynamical mean field theory is a powerful non-perturbative treatment of electron-electron interactions that is capable of capturing physics behond the one-electron approximiation, such as the Mott transition. In DMFT, one maps a lattice problem (Hubbard model, for example) to a single-site problem that is solved self-consistently. In this mapping, some information on spatial correlations are lost, but the temporal correlations are treated accurately. The main technical challenge is to solve the effective single-impurity problem. The bulk of this project was focused on this aspect.

To solve the single-impurity problem, a variety of methods were used: Exact diagonalization (ED), the non-crossing approximation (NCA), the one-crossing approximation (OCA), and continuous-time quantum monte carlo (CT-QMC). The latter is thought to be the most powerful and numerically accurate, but it can be computationally expensive. In this project, we compared the various solvers with each other for insulating and metallic systems, as well as for weak and strong coupling limits. We learned ED works best for metallic systems, and NCA/OCA works best for strongly coupled insulating systems. Therefore, NCA/OCA are natural solvers for strongly interacting topological insulator studies. Moreover, these techniques can require as little as 10% of the computing time as CT-QMC. So, a central result of this project is the expertise associate with this tool. This was the goal of the first year of this project; the second year was to be focused on the study of materials themselves. Nevertheless, we did make some progress in applying these methods to the physics of the Mott transition in a 2-orbital model relevant to nicklate films, and also the orbital polarization. Both of these are strongly influenced by electron interactions.

Other projects that received partial support from this grant were the discovery of a new interacting topological phase in three dimensions, TI*, the study of topological phases in thin-film transition metal oxides, and the first predictions of topological crystalline insulators in transition metal oxides. In addition, some quantum Monte carlo studies were carried out to investigate interaction effects on topological insulators in an ``unbaised'' manner. We found that the symmetry of the non-interacting terms in a Hamiltonian are decisive in whether interactions will stabilize or destabilize a topological phase, with higher symmetry (equal to lattice symmetry) favoring the topological phase.

All the major results cited above are contained in the various papers uploaded with this report.

Technology Transfer

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